Characterization of Mechanical Properties of Silica Aerogels

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Silica aerogels are nanoporous ultralight new materials with extraordinary material properties. In this study, the mechanical properties of silica aerogels, e.g. Young's modulus, Poisson's ratio and constitutive relation, are investigated using Molecular Dynamics (MD) simulations and theoretical analysis. In molecular dynamics simulations, an improved process of negative pressure rupturing method is adopted to generate more stable nano-porous structures of silica aerogels. Young's modulus and Poisson's ratio are measured by uniaxial and biaxial tension tests respectively. Our simulation results reveal that Young's modulus and Poisson's ratio of silica aerogels are both in a power-law relation to the density. According to the nano-porous structures, we propose a new theoretical ideal model for silica aerogels, and Young's modulus and Poisson's ratio are derived by continuum mechanics approach, assuming the backbone as a homogenous and isotropic material. Both simulation and theoretical prediction show a great identity. We hope this constitutive model can be used to investigate macro-mechanical property of silica aerogels in the future.

Keywords: Silica aerogels; Molecular dynamics simulations; Young's modulus; Poisson's ratio